Beach
10/694619

=> dis his

(FILE 'HOME' ENTERED AT 14:13:43 ON 13 DEC 2005)

FILE 'CASREACT' ENTERED AT 14:13:57 ON 13 DEC 2005
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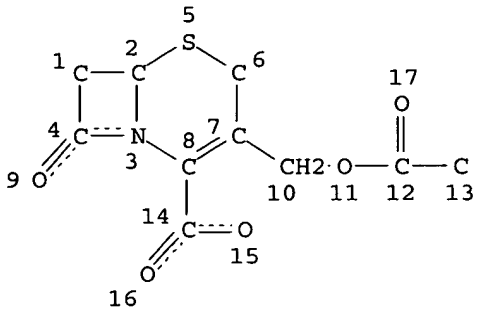
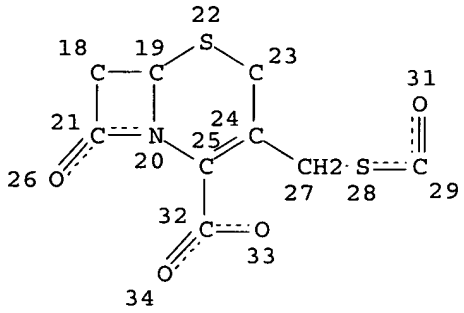
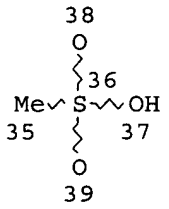
L3 STR L1
L4 1 S L3
L5 1 S L3 FUL

=> d l5 que stat;d fhit bib abs
L3 STR







2-sided

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE
L5 1 SEA FILE=CASREACT SSS FUL L3 (1 REACTIONS)

100.0% DONE 16 VERIFIED 1 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

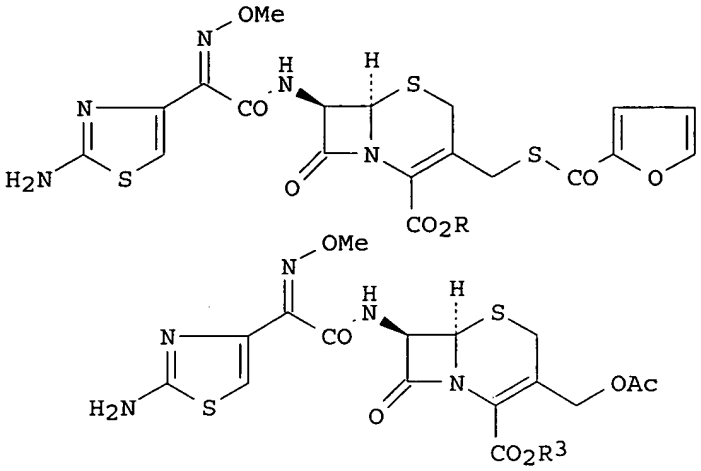
L5 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 1 **A** + B ===> **C**

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004132996	A1	20040708	US 2003-694619	20031027
PRAI	IN 2002-MU938	20021029			
OS	MARPAT 141:88965				
GI					

this work



I

AB A process for preparation of ceftiofur sodium I (R = Na) possessing high stability and having purity of more than 97% and substantially free of impurities, was disclosed. The process comprised reacting cefotaxime or its derivative II (R3 = H, alkali metal, alkaline earth metal, group forming an easily hydrolyzable ester) with 2-thiofuroic acid, employed in a molar proportion of 1.5 to 3.0 mol per mol of II, in the presence of acetonitrile as solvent and in the presence of large excess of methanesulfonic acid, employed in molar proportions of 12 to 18 mol per mol of II, and at a temperature of between -5° C. to 30° C. to give after necessary neutralization of the alkali or alkaline earth metal or removal of the ester group of the 4-carboxylic acid function, wherever applicable, ceftiofur I (R = H), possessing high stability and having purity of more than 97% and substantially free of impurities. Further,converting the ceftiofur to its salt with an organic amine by treating a solution of ceftiofur in a mixture of water and a water-miscible organic solvent with an organic amine, at a temperature ranging from -10° C. to 10° C., reacting of the amine salt thus obtained with a sodium metal carrier in a mixture of water and water-miscible organic solvent and in presence of sodium hydrogen sulfite to give the desired I (R = Na).

=> => dis his

(FILE 'HOME' ENTERED AT 14:13:43 ON 13 DEC 2005)

FILE 'CASREACT' ENTERED AT 14:13:57 ON 13 DEC 2005

L1 STR
L2 2 S L1
L3 STR L1
L4 1 S L3

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   242.07     242.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -0.68      -0.68

FILE 'REGISTRY' ENTERED AT 14:22:59 ON 13 DEC 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   12 DEC 2005  HIGHEST RN 869770-56-9
DICTIONARY FILE UPDATES:  12 DEC 2005  HIGHEST RN 869770-56-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> => dis his l16-;d l16 que stat;d l17 que stat;fil caplus;s (l19 or l20) and l17

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L17          469 S L14 FUL
L18        11557 S L16 OR L16
L19         2558 S L18  RAN=(,55371-13-6)
L20         9000 S L18  RAN=(55371-13-6,)


L10             STR



Prepared by: Mary Hale @2-2507 Rem Bldg 1D86
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	323.72	566.00

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.68

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 13 Dec 2005 VOL 143 ISS 25
FILE LAST UPDATED: 12 Dec 2005 (20051212/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

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          8924 L19
          7754 L20
           500 L17
L21        242 (L19 OR L20) AND L17
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L25       15649 S L24 OR L24
L26        6650 S L25  RAN=(,129695-40-5)
L27        9000 S L25  RAN=(129695-40-5,)
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FULL ESTIMATED COST	162.39	728.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.68

FILE 'CAPLUS' ENTERED AT 14:27:58 ON 13 DEC 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

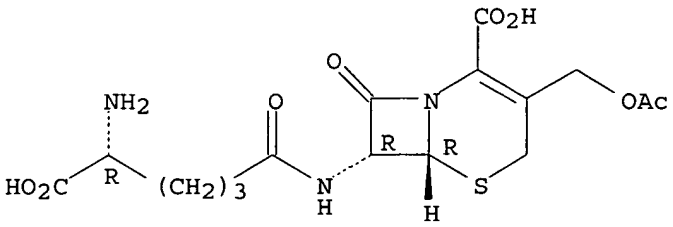
Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

nine of the most useful models for antimicrobial selection reported to date. Finally, a virtual screening of 87 new compds. reported in the anti-infective field with antibacterial activities is developed showing the ability of the models to identify new leads as antibacterial.

IT **61-24-5**, Cephalosporin C **153-61-7**, Cefalotin **804-53-5** **859-07-4**, Cefaloram **886-86-2**, Metacaine **1421-68-7**, Amidefrine mesylate **3577-01-3**, Cefaloglycin **8067-09-2**, Antibiotic 810A **23239-41-0**, Cefacetrile sodium **24356-60-3**, Cefapirin sodium **32178-82-8**, 7-(5-Amino-5-carboxyvaleramido)-7-methoxycephalosporanic acid **33075-00-2**, Cefathiamidine **34279-77-1**, Cephamycin B **36920-48-6**, Cefoxazole **39685-31-9**, Cefuracetime **51159-12-7**, Antibiotic BL-S217 **56083-50-2**, Antibiotic C-2801X **64485-93-4**, Cefotaxime sodium **69132-42-9**, Ceftioxide **69200-65-3** **80370-57-6**, Ceftiofur **82956-11-4**, Futhan **89201-82-1** **852448-72-7**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints as promising approach for modeling antibacterial activity)

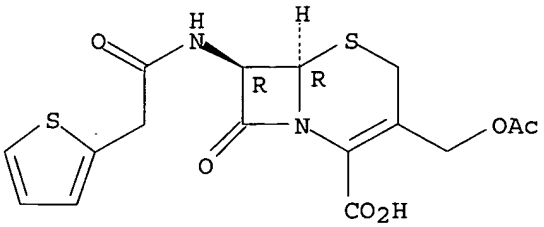
RN 61-24-5 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[(5R)-5-amino-5-carboxy-1-oxopentyl]amino]-8-oxo-, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153-61-7 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 804-53-5 CAPLUS
CN 2H-Benzo[a]quinolizin-2-one, 1,3,4,6,7,11b-hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-, (3R,11bR)-rel-, methanesulfonate (9CI) (CA INDEX NAME)

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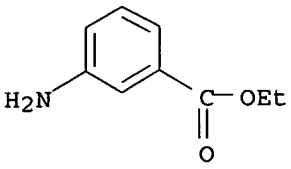
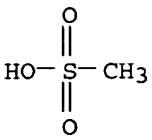


CM 2

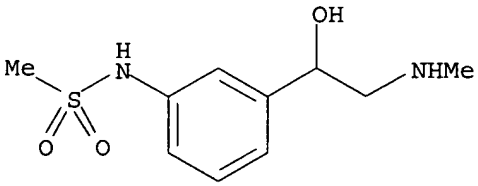
CRN 75-75-2
CMF C H4 O3 S



RN 1421-68-7 CAPLUS
CN Methanesulfonamide, N-[3-[1-hydroxy-2-(methylamino)ethyl]phenyl]-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 37571-84-9
CMF C10 H16 N2 O3 S



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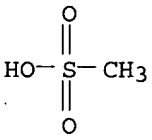
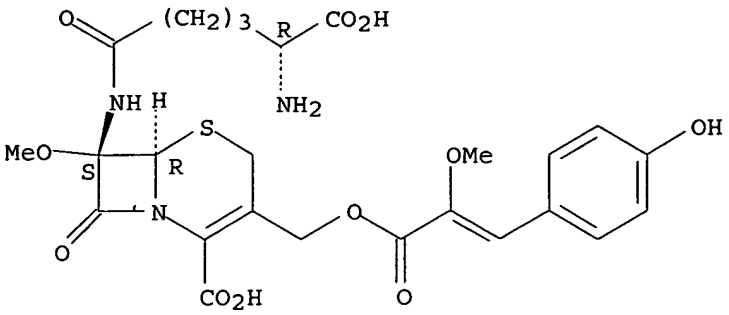


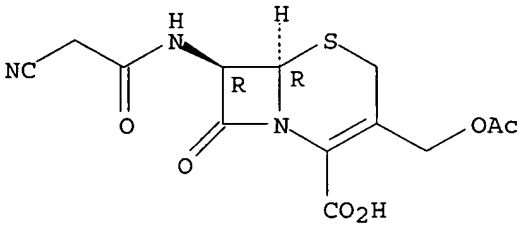
RN 3577-01-3 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[(2R)-aminophenylacetyl]amino]-8-oxo-, (6R,7R)-(9CI) (CA INDEX NAME)

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86



RN 23239-41-0 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[(cyanoacetyl)amino]-8-oxo-, monosodium salt, (6R,7R)- (9CI) (CA INDEX NAME)

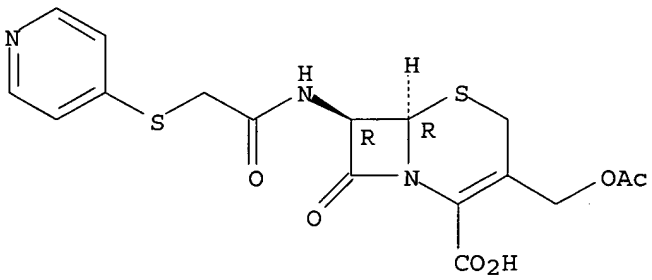
Absolute stereochemistry.



● Na

RN 24356-60-3 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-8-oxo-7-[[(4-pyridinylthio)acetyl]amino]-, monosodium salt, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

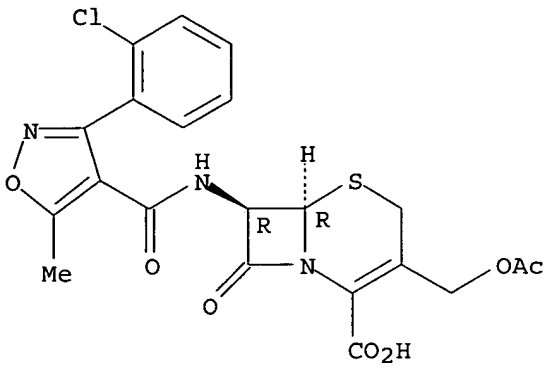


● Na

RN 32178-82-8 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

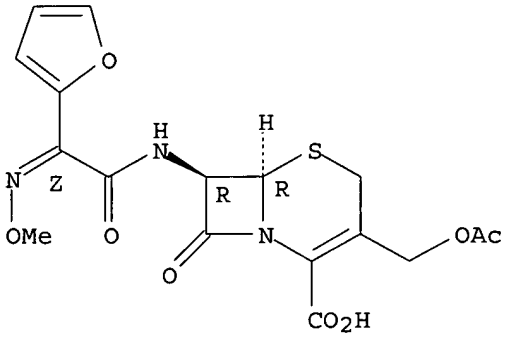
RN 36920-48-6 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[3-(2-chlorophenyl)-5-methyl-4-isoxazolyl]carbonyl]amino]-8-oxo-, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



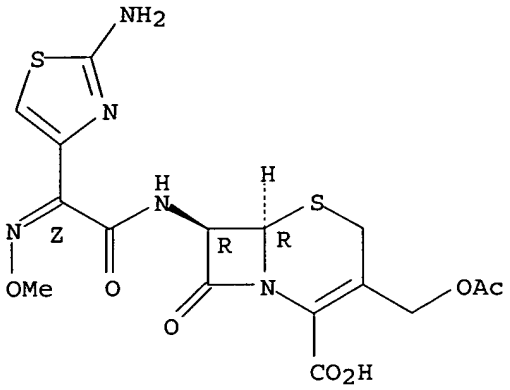
RN 39685-31-9 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[(2Z)-2-furanyl(methoxyimino)acetyl]amino]-8-oxo-, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 51159-12-7 CAPLUS
CN Pyridinium, 4-[[2-[[(6R,7R)-3-[(acetyloxy)methyl]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-7-yl]amino]-2-oxoethyl]thio]-1-methyl- (9CI) (CA INDEX NAME)

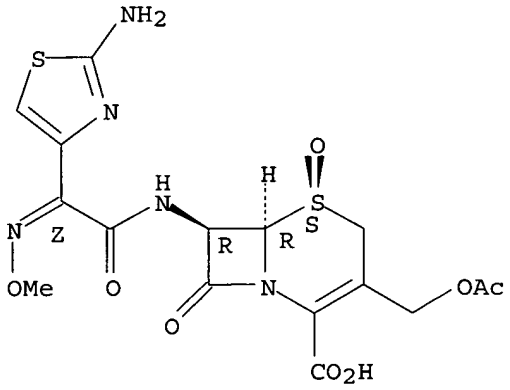
Absolute stereochemistry.



● Na

RN 69132-42-9 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[(2Z)-(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-8-oxo-, 5-oxide, (5S,6R,7R)- (9CI) (CA INDEX NAME)

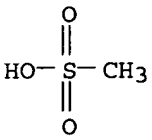
Absolute stereochemistry.
Double bond geometry as shown.



RN 69200-65-3 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[(5-amino-5-carboxy-1-oxopentyl)amino]-3-[[[3-(4-hydroxyphenyl)-2-methoxy-1-oxo-2-propenyl]oxy]methyl]-7-methoxy-8-oxo-, (6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

CRN 75-75-2
CMF C H4 O3 S

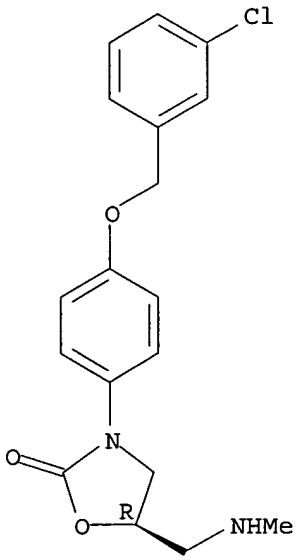


RN 89201-82-1 CAPLUS
CN 2-Oxazolidinone, 3-[4-[(3-chlorophenyl)methoxy]phenyl]-5-[(methylamino)methyl]-, (5R)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 84145-89-1
CMF C18 H19 Cl N2 O3

Absolute stereochemistry.



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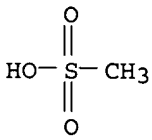

RN 852448-72-7 CAPLUS

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

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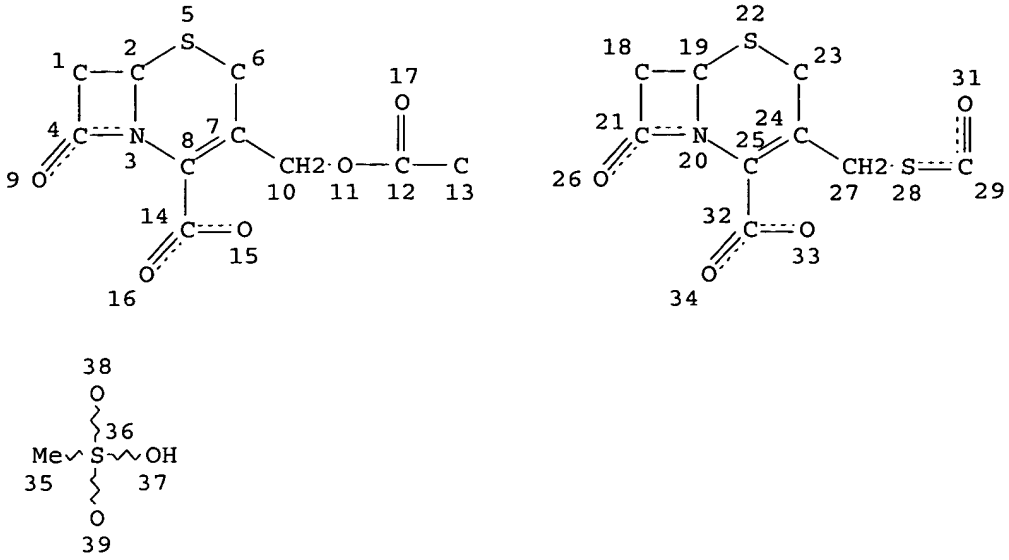

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE
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100.0% DONE 16 VERIFIED 1 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

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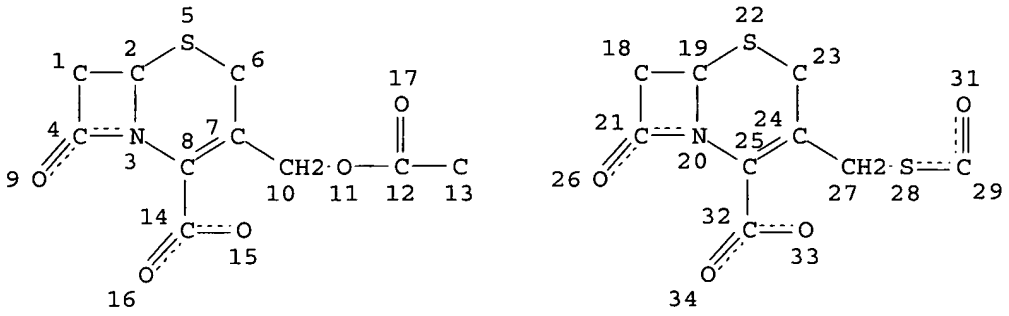

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

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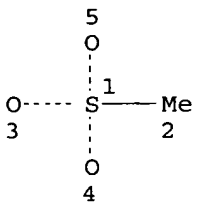

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 389720 ITERATIONS 15649 ANSWERS
SEARCH TIME: 00.00.04

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.84	734.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.73	-1.41

STN INTERNATIONAL LOGOFF AT 14:29:21 ON 13 DEC 2005